* Min Yu’s web site - <https://sites.google.com/site/minyuphys/resources>
* Paper: PRB 83 115113 (2011) (EDM), JCP 134 064111 (2011) (Bader charge integration)
* VASP version: 4.6.36 or 4.6.38 (I compiled EDM with vasp ver-4.6.38)
* Files from EDM calculation

1. OUTCAR: contains Ta, EXC, ECC integration and Enl per ion for every interation

##In the following, all the files beginning with 'EDM\_' are written in CHGCAR format.

2. EDM\_Ta: Kinetic energy density calculated using asymmetric form

3. EDM\_Tc: Kinetic energy density correction, difference of asymmetric and symmetric form

4. EDM\_exc: XC energy density

5. EDM\_VCCCAR: Total classical Coulomb potential\*(-1), (local pseudo-potential+ Hartree potential) used to define charge neutral volumes.

6. EDM\_VloCAR: Local pseudo-potential

7. EDM\_VhCAR: Hartree potential

8. EDM\_VmodCAR: Model potential

9. EDM\_neCAR: Valence electron = CHGCAR

10. EDM\_nmodCAR: Model charge density

11. EDM\_CHDEN: Soft pseudo-charge density used to define Bader volumes. (for PAW)

12. EDM\_CHGAUSS: Gaussian functional charge density used for USPP ions where EDM\_CHGAUSS is added into EDM\_CHDEN to define Bader volumes for individual ions.

~/vasp-tools/vtstscripts/chgsum.pl EDM\_CHDEN EDM\_CHGAUSS (for USPP)

13. EDM\_VnCAR: Total classical Coulomb energy density

* Energy integration using Bader charge (I use Dallas’s integration code)

bader EDM\_Ta -ref EDM\_CHDEN : gives atomic kinetic energy

bader EDM\_Tc -ref EDM\_CHDEN : gives kinetic energy integation error

bader EDM\_exc -ref EDM\_CHDEN : gives atomic xc energy

bader EDM\_VnCAR -ref EDM\_VCCCAR : gives atomic classic Coulomb energy

and nonlocal pseudo potential energy per atom is given in OUTCAR.

* INCAR file

LMAXMIX=4 (for convergence stability with d or f orbitals)

LELF = .TRUE.

NPAR = 1

LAECHG = .TRUE. (only for PAW)

NGX = 48; NGY = 640; NGZ = 432 (same with NGXF, NGYF, NGZF, EDM\_CHDEN file is written based on this grid points. For the energy integration, the number of grid of all EDM file have to be same)

NGXF= 48; NGYF= 640; NGZF= 432

* Calculation tips

Relax atoms 🡪 change the number of grid points as NGX = NGXF, one shot calculation to obtain WAVECAR and CHGCAR 🡪 read WAVECAR and CHGCAR and runs EDM calculation (help to converge)

Electronic energy convergence criteria is less than EDIFF = 0.1E-06 (eV)

Memory problem, check using makeparam, I mainly use ALGO = Normal instead of FAST due to memory problem